

ABSTRACT

METHOD FOR GENERATING A DATABASE OF MOLECULAR FRAGMENTS

5 A method is provided of generating a database of molecular fragment data defining parts of molecular structures, from a data set containing data describing predetermined molecular structures. The method comprises:-

- a) selecting first and second molecular structure data defining first and second molecular structures respectively from the data set;
- 10 b) comparing the selected data to determine molecular fragment data which defines at least part of a molecular structure common to each of the first and second molecular structures;
- c) storing the determined molecular fragment data in the data set; and,
- d) repeatedly performing steps (a) to (c) wherein either of the first or the
- 15 second molecular structure data is selected from either the predetermined molecular structure data or the molecular fragment data determined in step (b) such that the resultant data set comprises a database containing the molecular fragment data.